Manipulating molecules with mirrors: multi-scale molecular dynamics simulations of polaritonic chemistry

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When photoactive molecules interact strongly with confined light modes inside an optical cavity, new hybrid light-matter states can form, the so-called polaritons. These polaritons are coherent superpositions of excitations of the molecules and of the cavity photon. Recent experimental and theoretical works suggest that access to these polaritons in cavities might provide a totally new and attractive paradigm for controlling chemical reactions [1,2]. However, designing cavity parameters to control chemistry requires a theoretical model with which the effect of the light-matter coupling on the molecular dynamics can be predicted accurately. Therefore, we have developed a multi-scale quantum mechanics/molecular mechanics (QM/MM) molecular dynamics simulation model for photoactive molecules strongly coupled to confined light modes [3]. After presenting our model, I will show the results of simulations with thousands of molecules inside an optical cavity. These simulations illustrate how interaction with confined light affects the outcome of ultra-fast photochemical reactions. I will end the talk with a brief discussion of how strong coupling can be used for coherent light harvesting.

References

[1] Hutchison *et al*, Angew. Chem. Int. Ed., **51**, 1592 (2012)

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[3] Luk *et al*, J. Chem. Theory Comput. **13,** 77 (2017)